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Electron exchange by the CBO approximation in the excitation of helium-like positive ions by electron impact

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Calculation for electron exchange in the excitation of the helium-like positive ion by electron impact has been tackled through the Coulomb-Born-Oppenheimer (CBO) approximation. The integrals for the direct as also the exchange scattering amplitudes have been evaluated in a straight forward manner for any incident energy. Numerical results of the differential and total cross sections for the $1^1S \rightarrow 2^1S$ and the $1^1S \rightarrow 2^3S$ transitions in the particular ion Li^+ are given for the energy range from the threshold to five times the threshold.

1. Introduction

Electron collisional excitation of ions is a discipline of much interest and considerable attention to the physicists. The process of ionic excitation by electron impact plays an important role in various phenomena of astrophysics, plasma physics and atmospheric physics. Intensity analysis of certain spectral lines occurring in stellar radiations as well as electron temperature determination in hot plasma frequently depends on a good knowledge of excitation cross sections for scattering of electrons by ions. Helium-like ions turn convenient for use in the latter respect (Williams & Kaufman 1960). Moreover, such excitation cross sections for helium-like ions are useful for explaining the laboratory and astrophysical line spectra of the same ions (Gabriel & Jordan 1972).

Theoretical investigations by only a few authors exist as published results in the line of electron collisional excitation of helium-like positive ions. Sural and Sil have studied in the Coulomb-Born (CB) approximation the inelastic scattering of electrons by such positive ions and calculated for Li^+ the $1^1S \rightarrow 2^1S$ excitation cross section at threshold energy (Sural & Sil 1966) as also the $1^1S \rightarrow 2^1P$ excitation cross sections upto triplet the threshold energy (Sural & Sil 1969). Tully using the same approximation has investigated the electron impact excitations of Li^+, Be^{++} and O^{6+} for the transitions $1^1S \rightarrow n^1S$ and $1^1S \rightarrow n^1P$ with $n \leqslant 6$ (1974) and later on jointly with Serrao (1974), for the transitions $2^wS \rightarrow n^wS$ and $2^wS \rightarrow n^wP$ with $w = 1$ or 3, $2 < n \leqslant 6$ in the former case and $2 \leqslant n < 6$ in the latter. Both Sural & Sil and Tully have obtained, unlike the case of

neutral atom as target, finite nonzero threshold cross sections. But their values of threshold cross section for the $1^1S \rightarrow 2^1S$ excitation of Li^+ are not in agreement with each other. The anomaly has naturally brought us an incentive for a fresh investigation of the situation. Furthermore, the afore said authors have not taken into consideration the posibility of electron exchange which is supposed to play quite important a role in the transitions considered by them.

The scattering processes dealt with in the present paper are

$$X^{n+}(1^1S)+e^- \rightarrow X^{n+}(2^1S)+e^-$$

$$X^{n+}(1^1S)+e^- \rightarrow X^{n+}(2^3S)+e^-$$

where X^{n+} denotes a helium-like positive ion obtained by n fold ionization of the corresponding atom. Incidentally the transitions involving spin flip have also been considered by Beigman & Vainshtein (1967) and afterwards by Vainshtein (1974) alone in their method based on the use of orthogonalized functions. We, however, propose to tackle the calculation for electron exchange in the Coulomb-Born-Opponheimer approximation. The integral for scattering amplitude in the said approximation is evaluated in a straight forward way, quite a good number of the constituent integrals being worked out completely analytically and the others, reduced to suitable integrals for numerical evaluation.

2. Scattering Amplitudes in the CBO Approximation

The differential cross section for excitation by electron impact of a helium-like positive ion with nuclear charge Z from its ground state ψ_0 to the n-th state ψ_n is given as

$$I(\theta) = \frac{k_n}{k_0} |h|^2 \qquad \ldots (1)$$

with

$$h = \begin{cases} f, & \text{Singlet} \rightarrow \text{Singlet (CB)} \\ f-g, & \text{Singlet} \rightarrow \text{Singlet (CBO)} \\ g, & \text{Singlet} \rightarrow \text{Triplet} \end{cases} \qquad \ldots (2)$$

f and g being the amplitudes for scattering in direct and exchange channels respectively, given in atomic units by

$$f = -\frac{1}{2\pi} \int \psi_n^*(\boldsymbol{r}_1, \boldsymbol{r}_2)\chi(Z-2, -\boldsymbol{k}_n, \boldsymbol{r}_3)\left[-\frac{2}{r_3}+\frac{1}{r_{32}}+\frac{1}{r_{31}}\right]\psi_0(\boldsymbol{r}_1, \boldsymbol{r}_2)\times$$

$$\chi(Z-2, \boldsymbol{k}_0, \boldsymbol{r}_3)d\boldsymbol{r}_1\, d\boldsymbol{r}_2\, d\boldsymbol{r}_3 \qquad \ldots (3)$$

$$g = -\frac{C}{2\pi} \int \psi_n^*(\boldsymbol{r}_2, \boldsymbol{r}_3)\chi(Z-2, -\boldsymbol{k}_n, \boldsymbol{r}_1)[H-E]\psi_0(\boldsymbol{r}_1, \boldsymbol{r}_2)\times$$

$$\chi(Z-2, \boldsymbol{k}_0, \boldsymbol{r}_3)d\boldsymbol{r}_1\, d\boldsymbol{r}_2\, d\boldsymbol{r}_3. \qquad \ldots (4)$$

The χ's are the Coulomb wave functions corresponding to charge $Z-2$ and momentum vectors $\boldsymbol{k}_0$ and $-\boldsymbol{k}_n$, $\boldsymbol{k}_0$ and $\boldsymbol{k}_n$ being respectively the initial and final momenta of the electron. These have the form

$$\chi(Z, \boldsymbol{k}, \boldsymbol{r}) = \exp(\pi\nu/2)\Gamma(1-i\nu)\exp(i\boldsymbol{k}.\boldsymbol{r})_1F_1\{i\nu; 1; i(kr-\boldsymbol{k}.\boldsymbol{r})\} \tag{5}$$

with $\nu = Z/k$, ${}_1F_1$ representing the confluent hypergeometric function. In eq. (4), H is the hamiltonian of the system comprising the ion and an electron, E the total energy; C takes the value 1 for the singlet to singlet transition and $\sqrt{3}$ for the singlet to triplet. Here H being hermitian one can operate on either of the bound state functions $\psi_n^*(\boldsymbol{r}_2, \boldsymbol{r}_3)$ and $\psi_0(\boldsymbol{r}_1, \boldsymbol{r}_2)$ in eq. (4). Accordingly one obtains, by making use of the eigenvalue equation for the corresponding bound state of the ion,

$$g = \frac{C}{2\pi} \int \psi_n^*(\boldsymbol{r}_2, \boldsymbol{r}_3)\chi(Z-2, -\boldsymbol{k}_n, \boldsymbol{r}_1)\left[-\frac{2}{r_j} + \frac{1}{r_{j2}} + \frac{1}{r_{13}}\right] \times$$

$$\psi_0(\boldsymbol{r}_1, \boldsymbol{r}_2)\chi(Z-2, \boldsymbol{k}_0, \boldsymbol{r}_3)d\boldsymbol{r}_1\, d\boldsymbol{r}_2\, d\boldsymbol{r}_3 \tag{6}$$

in which j is 1 for the post interaction and 3 for the prior (result of operation on ψ_n^* and ψ_0 respectively).

In obtaining eq. (6), ψ_n and ψ_0 have been assumed to be exact wave functions. However, in practice these state functions are approximate and do not satisfy the eigenvalue equation exactly. As a consequence, results with post and prior interactions might differ from each other, which is known as the post-prior discrepancy.

3. Wave Functions of the Helium-Like Ion

Enormous saving of labour is achieved in the analytical portion of our calculation by employing simple target wave functions. Analytic functions given by Morse *et al* (1935) for the ground state and singlet and triplet $2S$ states of helium-like ions are indeed adequately simple in form. Still it remains to be worth mentioning, while the ground 1^1S and the excited 2^3S state functions are mutually orthogonal the 2^1S state wave function of Morse *et al* does not satisfy the condition of orthogonality with the ground state function. So we like to adopt for the 1^1S and 2^3S states the wave functions of Morse *et al* but intend to construct in simple form the 2^1S state function ensuring that it is orthogonal to the ground state wave function.

The ground 1^1S and excited 2^3S state functions of Mrose *et al* are given as

$$\psi_{1^1S}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \frac{(a'\mu')^3}{\pi} \exp\{-a'\mu'(r_1+r_2)\} \quad \ldots \quad (7)$$

$$\psi_{2^3S}(r_1, r_2) = \frac{1}{\sqrt{2}} \left(\frac{a^3\mu^3}{\pi}\right)^{\frac{1}{2}} \left(\frac{\mu^5}{3\pi N}\right)^{\frac{1}{2}} \left[\exp(-a\mu r_1)\left\{r_2 \exp(-\mu r_2) - \frac{3A}{\mu}\exp(-b\mu r_2)\right\} - \exp(-a\mu r_2)\left\{r_1 \exp(-\mu r_1) - \frac{3A}{\mu}(\exp - b\mu r_1)\right\}\right] \quad \ldots (8)$$

with

$$A = \frac{(a+b)^3}{(1+a)^4} \quad \text{and} \quad N = 1 - \frac{48A}{(1+b)^4} + \frac{3A^2}{b^3}$$

The numerical values of $a'\mu'$ and $a, a\mu, b, b\mu$ and 2μ for a number of positive ions belonging to the helium isoelectronic sequence are tabulated in the said paper.

To construct the 2^1S state wave function we have carried out variational calculations for the eigen energy imposing the condition of orthogonality between this and the ground state wave function of Morse *et al* given above. The 2^1S state function thus obtained is cast into a form similar to that in eq. (8) in order to facilitate a common program to be made for both 2^1S and 2^3S excitations. So we write

$$\psi_{2^1S}(r_1, r_2) = \frac{1}{\sqrt{2}} \left(\frac{a^3\mu^3}{\pi}\right)^{\frac{1}{2}} \left[\frac{\mu^5}{3\pi N(1+\Delta^2)}\right]^{\frac{1}{2}} \left[\exp(-a\mu r_1) \times \left\{r_2 \exp(-\mu r_2) - \frac{3A}{\mu}\exp(-b\mu r_2)\right\} + \exp(-a\mu r_2) \times \left\{r_1 \exp(-\mu r_1) - \frac{3A}{\mu}\exp(-b\mu r_1)\right\}\right]. \quad \ldots (9)$$

Here A does not carry the same definition as in eq. (8) and is now obtained from the condition of orthogonality between the 1^1S and 2^1S wave functions as a whole. The quantity Δ (its value is non-zero) comes because of the nonorthonality between the $1s$ and $2s$ orbitals that build up our wave function. In fact Δ is the over lap integral between these two orbitals (c.f. Marriott & Seaton 1957). Finally N in eq. (9) is related to the normalization constant for the $2s$ orbital. The numerical values of the parameters μ, $b\mu$ and the derived quantities like A, N and Δ for a number of helium-like positive ions have been calculated in course of our construction of the 2^1S state function, $a\mu$ being merely the charge of the ion.

4. Evaluation of the Integrals for the Scattering Amplitudes

Use is made of the integral representation (Das *et al* 1976) for the confluent hypergeometric function ${}_1F_1$ in eq. (5), so that the scattering amplitudes can be written out as

$$f = C_2 J_D \quad \text{and} \quad g = C_2(J_{E_1} + J_{E_2}) \qquad \ldots \quad (10)$$

where

$$C_2 = \frac{1}{\sqrt{2}} \frac{(a'\mu')^3}{\pi^3} \left[(a\mu)^3 \frac{\mu^5}{3N(1+\Delta^2)} \right]^{\frac{1}{4}} \exp\{\pi(\alpha+\alpha_0)/2\}\Gamma(1-i\alpha_0)\Gamma(1-i\alpha) \qquad \ldots \quad (11)$$

where $\alpha = (Z-2)/k_n$, $\alpha_0 = (Z-2)/k_0$, Δ being zero for the $1^1S \rightarrow 2^3S$ transition; J_D, J_{E_1} and J_{E_2} are given by

$$J_D = \frac{1}{4\pi^2} \oint_\Gamma \oint_{\Gamma_0} dt_1\, dt_2\, p(t_1, \alpha_0) p(t_2, \alpha) \int d\boldsymbol{r}_1\, d\boldsymbol{r}_2\, d\boldsymbol{r}_3\, F(\boldsymbol{r}_3) \left[-\frac{1}{r_3} + \frac{1}{r_{13}} \right]$$

$$\times \left[-\frac{3A}{\mu} \exp(-\lambda_1 r_1 - \lambda_3 r_2) - \frac{3A}{\mu} \exp(-\lambda_3 r_1 - \lambda_1 r_2) \right.$$

$$\left. + r_1 \exp(-\lambda_2 r_1 - \lambda_1 r_2) + r_2 \exp(-\lambda_1 r_1 - \lambda_2 r_2) \right] \qquad (12)$$

in which

$$F(\boldsymbol{r}_3) = \exp[i(\boldsymbol{k}_0 - \boldsymbol{k}_n).\boldsymbol{r}_3 + i(k_n r_3 + \boldsymbol{k}_n.\boldsymbol{r}_3)t_2 + i(k_0 r_3 - \boldsymbol{k}_0.\boldsymbol{r}_3)t_1] \qquad (13)$$

$$J_{E_1} = \frac{C}{8\pi^2} \oint_\Gamma \oint_{\Gamma_0} dt_1\, dt_2\, p(t_1, \alpha_0) p(t_2, \alpha) \left[-\frac{3A}{\mu} \{-2U_f(a'\mu', \lambda_1, b\mu) \right.$$

$$+ V_f(a'\mu', \lambda_1, b\mu)\} + B_1\{-2U_f(a'\mu', \lambda_3, a\mu) + V_f(a'\mu', \lambda_3, a\mu)\}$$

$$- \left\{ -2 \frac{\partial}{\partial\mu} U_f(a'\mu', \lambda_1, \mu) + \frac{\partial}{\partial\mu} V_f(a'\mu', \lambda_1, \mu) \right\}$$

$$\left. - B_2 \left\{ -2 \frac{\partial}{\partial\lambda_2} U_f(a'\mu', \lambda_2, a\mu) + \frac{\partial}{\partial\lambda_2} V_f(a'\mu', \lambda_2, a\mu) \right\} \right]. \qquad \ldots \quad (14)$$

$$J_{E_2} = \frac{C}{8\pi^2} \oint_\Gamma \oint_{\Gamma_0} dt_1\, dt_2\, p(t_1, \alpha_0) p(t_2, \alpha) \left[-\frac{3A}{\mu} W(a'\mu', \lambda_1, b\mu) \right.$$

$$\left. + B_1 W(a'\mu', \lambda_3, a\mu) - \frac{\partial}{\partial\mu} W(a'\mu', \lambda_1, \mu) + B_2 \frac{3}{\lambda_2} W(a'\mu', \lambda_2, a\mu) \right] \qquad \ldots \quad (15)$$

with

$$U_j(\mu_1, \mu_2, \mu_3) = \int d\boldsymbol{r}_1\, d\boldsymbol{r}_2\, d\boldsymbol{r}_3 \frac{F_1(\boldsymbol{r}_1, \boldsymbol{r}_3)}{r_j} \exp(-\mu_1 r_1 - \mu_2 r_2 - \mu_3 r_3) \quad \ldots (16)$$

$$V_j(\mu_1, \mu_2, \mu_3) = \int d\boldsymbol{r}_1\, d\boldsymbol{r}_2\, d\boldsymbol{r}_3 \frac{F_1(\boldsymbol{r}_1, \boldsymbol{r}_3)}{r_{j_2}} \exp(-\mu_1 r_1 - \mu_2 r_2 - \mu_3 r_3) \quad \ldots (17)$$

$$W(\mu_1, \mu_2, \mu_3) = \int d\boldsymbol{r}_1\, d\boldsymbol{r}_2\, d\boldsymbol{r}_3 \frac{F_1(\boldsymbol{r}_1, \boldsymbol{r}_3)}{r_{13}} \exp(-\mu_1 r_1 - \mu_2 r_2 - \mu_3 r_3) \quad \ldots (18)$$

$$F_1(\boldsymbol{r}_1, \boldsymbol{r}_3) = \exp[i(\boldsymbol{k}_0 \cdot \boldsymbol{r}_3 - \boldsymbol{k}_n \cdot \boldsymbol{r}_1) + i(k_n r_1 + \boldsymbol{k}_n \cdot \boldsymbol{r}_1)t_2 + i(k_0 r_3 - \boldsymbol{k}_0 \cdot \boldsymbol{r}_3)t_1)] \quad \ldots (19)$$

B_1 and B_2 are respectively $-3A/\mu$ and 1 for the $1^1S \rightarrow 2^1S$ excitation while for the $1^1S \rightarrow 2^3S$ transition they are $3A/\mu$ and -1 taken in like order. $\lambda_1, \lambda_2, \lambda_3$ in eqs. (12), (14) and (15) are but different combinations of the wave function parameters such that

$$\lambda_1 = a'\mu' + a\mu, \quad \lambda_2 = a'\mu' + \mu, \quad \lambda_3 = a'\mu' + b\mu$$

and finally, $t^{-1+ix}(t-1)^{-ix}$ is the form of the function $p(t, x)$ involved.

Now the integrals in J_D are either of the type

$$K = -\frac{1}{4\pi^2} \oint_\Gamma \oint_{\Gamma_0} dt_1\, dt_2\, p(t_1, \alpha_0) p(t_2, \alpha) \int d\boldsymbol{r}_1\, d\boldsymbol{r}_2\, d\boldsymbol{r}_3\, F(\boldsymbol{r}_3) \times \left[-\frac{1}{r_3} + \frac{1}{r_{13}}\right] \exp(-\mu_1 r_1 - \mu_2 r_2) \quad \ldots (20)$$

or obtainable from it by ere parametric differentiation. To evaluate K the space integrations are first carried out. This leaves us in eq. (20) with the t_1, t_2 complex double integrals of which the t_2 integration* is done analytically by residue calculation at the pole. Thus we are led to

$$K = -\frac{1}{2\pi i} \oint_{\Gamma_0} dt_1\, p(t_1, \alpha_0) V(t_1) \quad \ldots (21)$$

where the function $V(t_1)$ has the form

$$V(t_1) = -\frac{64\pi^2}{\mu_1^3 \mu_2^3} \left[J(t_1) - \frac{\mu_1}{2} \frac{\partial}{\partial \mu_1} J(t_1) \right] \quad \ldots (22)$$

with

$$J(t_1) = \frac{2\pi}{k_n - k_0(1-t_1)\cos\theta + k_0 t_1 + i\mu_1} \left[1 - \frac{k_n}{x}\right]^{-t_\alpha} \cdot \frac{1}{x} \quad (23)$$

* Here the t_1 integration could instead be done but the alternative has been preferred since this enables us to pursue the calculation even at the threshold energy for which k_n is zero.

θ being the scattering angle and

$$x = \frac{-k_0^2(1-2t_1)-k_n^2+2\boldsymbol{k}_0.\boldsymbol{k}_n(1-t_1)-\mu_1^2+2i\mu_1 t_1 k_0}{-2k_n+2k_0(1-t_1)\cos\theta-2k_0 t_1-2i\mu_1} \quad \ldots (24)$$

The complex t_1 integration in eq. (21) is finally done numerically following the method of Mukherjee *et al* (1975) with a slight modification.

As for the evaluation of J_{E_1}, the complex t_1, t_2 integrals in eq. (14) do not involve the scattering angle and are separable. The complex t integrals that we come across after separation can indeed be expressed out in terms of the integral of type

$$I(\beta, k, \mu_1) = \frac{1}{2\pi i}\oint_{\Gamma} dt\, p(t,\beta)\int d\boldsymbol{r}\, e^{-\mu_1 r}\exp\{i(kr\mp\boldsymbol{k}.\boldsymbol{r})t\mp i\boldsymbol{k}.\boldsymbol{r}\}. \quad \ldots (25)$$

The space integral in eq. (25) is a standard one and the complex t integration is done by calculating the residue at the pole. Thus I is reduced to

$$I(\beta, k, \mu_1) = \frac{4\pi\exp(-\beta\theta_1)}{k^2+\mu_1^2} \quad \ldots (26)$$

with

$$\theta_1 = \tan^{-1}\{2\mu_1 k/(\mu_1^2-k^2)\}. \quad \ldots (27)$$

Lastly, evaluation of J_{E_2} only requires consideration of the type integral

$$L = -\frac{1}{4\pi^2}\oint_{\Gamma}\oint_{\Gamma_\alpha} dt_1\, dt_2\, p(t_1,\alpha_0)p(t_2,\alpha)W(\mu_1,\mu_2,\mu_3). \quad (28)$$

As already shown by us the integral L can be reduced to the form

$$L = \frac{1}{2\pi i}\oint_{\Gamma}\int_{-1}^{1} dt_1\, dz_1\, p(t_1,\alpha_0)V_1(t_1,Z_1) \quad (29)$$

in which

$$V_1(t_1,Z_1) = \frac{64\pi^3}{\mu_2^3}\frac{\partial^2 V'(t_1,Z_1)}{\partial\mu_1\partial\mu_3} \quad (30)$$

Here $V'(t_1, Z_1)$ is given explicitly by

$$V'(t_1,Z_1) = -\left[\frac{G\left(1-\frac{k_n}{F}\right)^{-i\alpha}(x_1+y_1F)-F\left(1-\frac{k_n}{G}\right)^{-i\alpha}(x_1+y_1G)}{FG\xi(F-G)}\right] \quad (31)$$

with

$$x_1 = (\mu_3-ik_0t_1)(k_n^2+\mu_1^2)+\mu_1\{k_0^2(1-2t_1)+\mu_3^2-2i\mu_3k_0t_1\},$$

$$y_1 = -[2(k_n+i\mu_1)(\mu_3-ik_0t_1)+i\{k_0^2(1-2t_1)+\mu_3^2-2i\mu_3k_0t_1\}],$$

$$\xi = y_1^2(1-Z_1^2)-2y_2y_4(k_n+i\mu_1)Z_1^2,$$
$$y_2 = -2k_n+2k_0(1-t_1)\,\mathrm{Cos}\,\theta-2i(\mu_1+\mu_3)-2k_0t_1,$$
$$y_4 = k_0^2(1-2t_1)+\mu_3^2-2i\mu_3k_0t_1,$$
$$F = (-y-\sqrt{y^2-4x\xi})/2\xi,$$
$$G = (-y+\sqrt{y^2-4x\xi})/2\xi,$$
$$x = x_1^2(1-Z_1^2)+x_2y_4(k_n^2+\mu_1^2)Z_1^2,$$
$$x_2 = k_n^2+k_0^2(1-2t_1)-2\boldsymbol{k}_0.\boldsymbol{k}_n(1-t_1)+(\mu_1+\mu_3)^2-2ik_0t_1(\mu_1+\mu_3),$$
$$y = 2x_1y_1(1-Z_1^2)+\{y_2(k_n^2+\mu_1^2)-2x_2(k_n+i\mu_1)\}y_4Z_1^2.$$

The double integral L in eq. (29) is evaluated numerically, the complex t_1 integration being done as before.

In the numerical computation, it must be pointed out, the functions of the form $\left(1-\frac{k_n}{u}\right)^{-i\alpha}$ in eqs. (23) and (31) and the expression $\exp(-\beta\theta_1)$ with $\beta=\alpha$ in eq. (26) exhibit indeterminacy at the threshold energy (k_n is zero). This difficulty is got rid of by taking the limits of the said quantities as k_n tends to zero which turn out to be $\exp\{i(Z-2)u\}$ and $\exp\{-2(Z-2)/\mu_1\}$ respectively.

5. Scattering Cross Sections

Evaluation of J_D, J_{E_1} and J_{E_2} being done the additional requirement for the estimation of differential cross section from eq. (1) is only to evaluate the quantity $k_n|C_2|^2/k_0$ which is found to be

$$\frac{k_n}{k_0}\cdot\frac{(a'\mu')^6(a\mu)^3\mu^5}{6N(1+\Delta^2)\pi^6}\exp\{\pi(\alpha+\alpha_0)\}\frac{\pi\alpha_0}{\mathrm{Sinh}(\pi\alpha_0)}\cdot\frac{\pi\alpha}{\mathrm{Sinh}(\pi\alpha)}\cdot$$

For computing the threshold differential cross section, however, we need to take the limit of the said quantity as k_n tends to zero; this limit becomes

$$\frac{(a'\mu')^6(a\mu)^3\mu^5(Z-2)\alpha_0\exp(\pi\alpha_0)}{3N(1+\Delta^2)\pi^4k_0\,\mathrm{Sinh}\,(\pi\alpha_0)}.$$

The evaluation of $2\pi\int_0^\pi I(\theta)\,\mathrm{Sin}\,\theta\,d\theta$ is now performed to obtain the total cross section for the excitation of the helium-like ion.

6. Results and Discussion

6.1 $1^1S\rightarrow 2^1S$ *excitation of* Li^+

Computation has been carried out for the differential and total cross sections in the energy range between threshold and five times the threshold

taking the calculated values of Morse *et al* for the 1^1S state eigenenergy and the parameter $(a'\mu')$ together with the values of eigenenergy $\epsilon(2^1S)$, parameters $a\mu$, $b\mu$, μ and derived quantities A, N, Δ as obtained by ourselves (quoted below) for the 2^1S state.

$\epsilon(2^1S) = -5{\cdot}038229$ a.u., $a\mu = 3{\cdot}0$, $b\mu = 1{\cdot}55709$,
$\mu = 0{\cdot}99975$, $A = 0{\cdot}41322$, $N = 0{\cdot}67196$,
$\Delta = 0{\cdot}04039$.

In figure 1, are depicted our results for the differential cross sections in CB and CBO approximations at threshold energy 59·4122 eV. CBO results are given with both post and prior interactions. It is seen the two CBO curves at threshold lie well above the CB one, the cross section with post interaction being larger than that with prior at all angles. The CB and CBO differential cross sections rise from the lowest value at 0° upto a maximum at 180°. The effect of electron exchange is rather pronounced at this energy over the entire range of scattering angle.

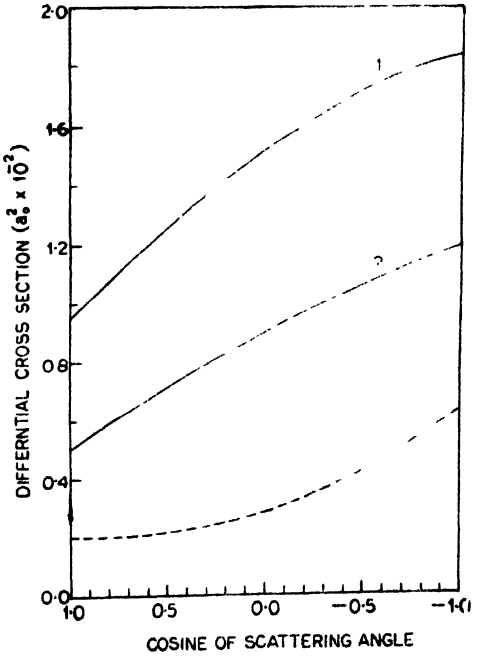

Fig. 1. $1^1S \rightarrow 2^1S$ excitation of Li^+ under electron impact at threshold energy (59·4122 eV), Dotted curve, CB; solid curves 1 and 2, CBO with post and prior interactions respectively.

From double the threshold onwards, the differential graph exhibits more or less an identical feature, which is true for the CB as well as CBO approximation. At these energies, unlike the threshold case, CB and CBO differential

cross sections show their maximum values at 0°, thereafter they start falling down gradually to reach the lowest point in the differential curve at 180°; the said fall, however, gets faster with increasing incident energy. Moreover, contrary to the situation at threshold, the post curve now lies below the prior until the two merge into a single in the small angle region. It would be quite interesting to note, at energies other than the threshold CB and CBO make hardly any effective difference in the result for differential cross section at small angles. For illustration we present here double the threshold differential graphs (figure 2).

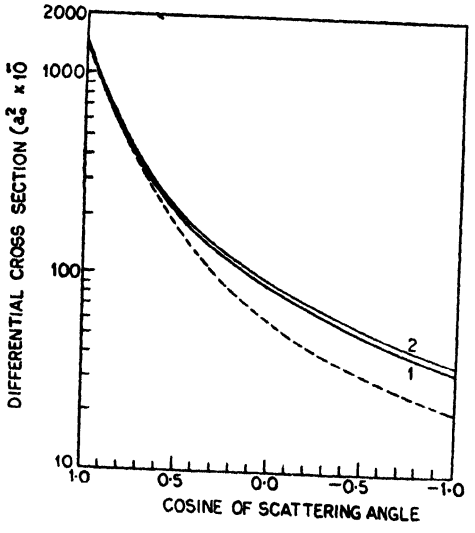

Fig. 2. $1^1S \rightarrow 2^1S$ excitation of Li^+ under electron impact at double the threshold energy (118·824 eV). Dotted curve, CB; solid curves 1 and 2, CBO with post and prior interactions respectively.

Our total cross section results at energies within the mentioned range are shown in table 1. Unfortunately there exist no measurements for a possible comparative study to be made with. The table contains in addition to the CB and CBO cross sections in the present investigation, the CB cross section values due to Tully obtained in the partial wave analysis with many parameter wave functions (McEachran & Cohen 1969) employed for the target states as also the CB threshold cross section of Sural & Sil (1966) who have used the wave functions given by Morse *et al.* We have come to know through private communication about the CBO calculations done very recently in the partial wave analysis by McDowell *et al* (1976) for the excitation of the helium-like positive ion with the use of McEachran and Cohen wave functions. The CB and CBO total cross sections obtained by them for Li^+ at 62·56 eV, an incident energy very near the threshold are $15{\cdot}86 \times 10^{-3}\ \pi a_0^2$ and $42{\cdot}63 \times 10^{-3}\ \pi a_0^2$ respectively.

Incidentally the results of McDowell *et al* are obtained right from eq. (4) by substitution of the expressions for the 1^1S and 2^1S state functions therein, without exploiting the eigenvalue equation for the bound state of the ion. So in their case the question of post-prior discrepancy does not arise.

Clearly the difference between CB and CBO total cross section values at threshold is highly appreciable. At other energies the exchange effect seems to be persisting in a presumably reduced manner.

The CB total cross sections in the present study appear to be in fairly good agreement with those of Tully given upto triple the threshold energy. The discrepancy that exists between the two results is not very unlikely in view of the fact that Tully has employed many parameter wave functions of McEachran and Cohen while ours are the simple 1^1S state wave function of Morse *et al* and the 2^1S state function constructed by ourselves in adequately simple form.

The threshold total CB cross section for Li^+ due to Sural & Sil (1966) is too low, as shown by table 1, compared to our value for the same as well as the corresponding result of Tully. For a clarification on this point we have also calculated the threshold cross section (CB) using the initial and final state functions both

Table 1. Total cross sections in $\pi a_0^2 \times 10^{-3}$ unit for $1^1S \rightarrow 2^1S$ excitation of Li^+ by electron impact.

Incident energy in threshold unit	CB			CBO	
	Sural & Sil	J.A. Tully*	Present	Post	Prior
1	3·04	16·80	13·30	59·20	35·50
2	—	9·34	6·99	7·80	8·05
3	—	6·45	4·76	4·31	4·54
4	—	—	3·61	3·18	3·29
5	—	—	2·90	2·57	2·63

* Threshold energy is 60·05 eV,

given by Morse *et al*, with the electron-nucleus term of the potential retained as also that omitted in the calculation. The corresponding differential cross section curves (1a and 1b respectively) are presented in figure 3 which as well contains that (curve 2) obtained in our actual calculation where the 2^1S state function constructed by ourselves has been used. The total cross sections obtained with and without retaining the said electron-nucleus term are found to be $33{\cdot}6 \times 10^{-3}\ \pi a_0^2$ and $3{\cdot}04 \times 10^{-3}\ \pi a_0^2$ respectively. We see, the differential cross section curve and the total cross section value of Sural and Sil have been exactly reproduced in our calculation with 1^1S and 2^1S state functions of Morse

et al, if of course, the electron-nucleus term is omitted. This shows, the calculation of Sural and Sil who have taken the wave functions of Morse *et al* to be mutually orthogonal is free from any numerical error. However, the use of the non-orthogonal set of 1^1S and 2^1S wave functions due to Morse *et al* is not justified

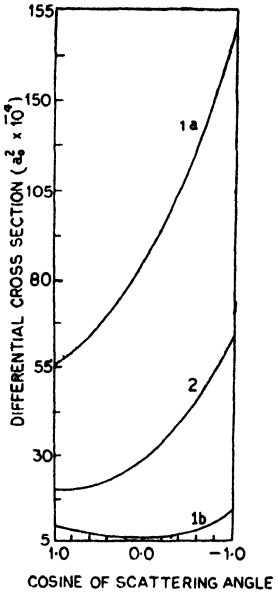

Fig. 3. Threshold differential corsssection (CB) for $1^1S \rightarrow 2^1S$ excitation of Li^+ by electron impact to illustrate the effect on the result, of non-orthogonality between initial and final state functions. Curves 1a and 1b, obtained by using 1^1S and 2^1S state functions of Morse *et al* with the electron-nucleus interaction term respectively retained and omitted in calculation; curve 2, obtained by using the constructed 2^1S state wave function that is orthogonal to the ground 1^1S state function of Morse *et al*.

considering the large difference between the results, calculated with and without the electron-nucleus interaction term. But we do not understand how Tully using the same target wave functions as done by Sural and Sil has obtained a different result.

6.2 $1^1S \rightarrow 2^3S$ *excitation of* Li^+

The differential and total cross sections have been estimated as earlier in the threshold-to-five times threshold energy range. In this case we have used the experimental values for the 1^1S and 2^3S state eigenenergies as quoted by Morse *et al* and the threshold energy is 59·0104 eV.

Here too, one sees as in the case of $1^1S \rightarrow 2^1S$ excitation, the general behaviour of the differential cross section curve at threshold is quite different from the same at other energies considered in the specific range. We present the relevant graphs in figures 4 and 5 for threshold and five times the threshold respectively.

The threshold differential cross section rises from the lowest value at 0° to attain a broad maximum, then it gradually falls down. The prior curve at this energy floats all along above the post (figure 4).

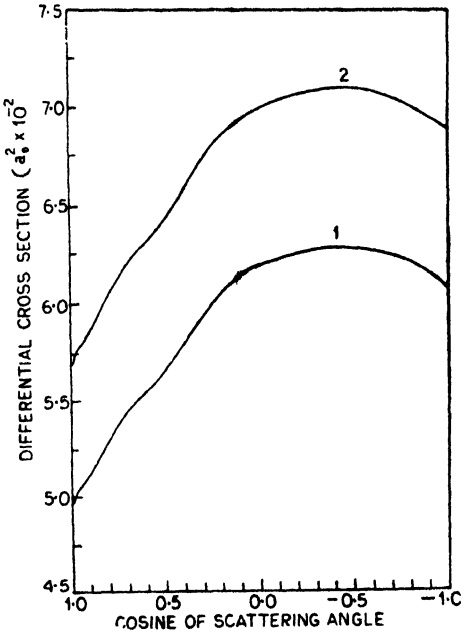

Fig. 4. $1^1S \rightarrow 2^3S$ transition in Li^+ by electron impact at threshold energy (59·0104 eV) in CBO approximation. Curve 1, Post interaction; curve 2, prior interaction.

Opposed to the threshold case, the differential cross section from double the threshold ahead, has its largest value at 0°. The cross section curve at double as well as triple the threshold shows a minimum, its position being shifted towards 0° in the latter case (not shown in figure). It is of interest to find at four and five times the threshold, there occur in the differential curve two minima resulting in a kink that is rather large at the higher energy. Finally, the cross section with post interaction at energies other than threshold is more than that with prior (see for example figure 5).

In table 2, are presented our total cross section results at the incident energies said above. Here also we do not find any experimental result for comparison. Preliminary results for the differential and total cross sections at double the threshold have already been reported (Das *et al* 1976). For the sake of completeness these results are included here too.

The results obtained by Beigman & Vainshtein (1967) for Li^+ in their method based on the use of orthogonalized functions are incorrect. The correct result in this method has, however, been given by Vainshtein (1974) and yields a

threshold cross section of $0{\cdot}41\times10^{-3}\ \pi a_0^2$. This is more than 500 times smaller than the result obtained here in the CBO approximation.

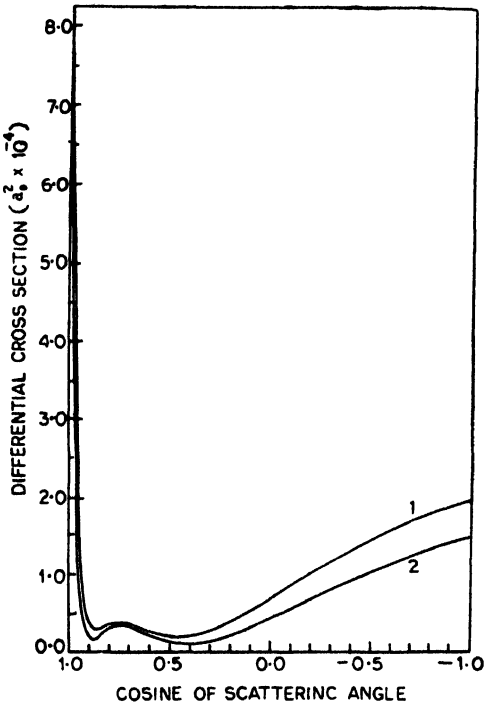

Fig. 5. $1^1S \rightarrow 2^3S$ transition in Li^+ by electron impact at five times the threshold energy (295·052 eV) in CBO approximation. Curve 1, post interaction; curve 2, prroi interaction.

Table 2. Total cross sections in $\pi a_0^2\times10^{-3}$ unit for $1^1S \rightarrow 2^3S$ excitation of Li^+ by electron impact.

Incident energy in threshold unit.	CBO	
	Post	Prior
1	238·00	269·00
2	18·70	17·10
3	3·28	2·78
4	0·904	0·731
5	0·389	0·284

One sees from table 2 that the total cross section in CBO approximation for the $1^1S \rightarrow 2^3S$ transition in Li^+ is very high at the threshold energy. In

fact this value is much larger than the corresponding one for the $1^1S \rightarrow 2^1S$ excitation. At double the threshold too, the value of total cross section for such transition is more by an appreciable amount than that at the corresponding energy for the $1^1S \rightarrow 2^1S$ excitation. Nevertheless, the $1^1S \rightarrow 2^3S$ excitation cross section for Li^+ as evident from table 2 falls off very fast with increasing incident energy.

7. Conclusion

The Coulomb-Born-Oppenheimer method is a weak coupling approximation that treats the electron-electron interaction as a small perturbation and allows for the distortion of the colliding electron's motion only by the long range Coulomb field of the ion. It makes allowance for electron exchange which is very important at low energy but the approximation itself does not seem to be very reliable near the threshold specially for the $S \rightarrow S$ transitions. However, at higher energies the CBO is expected to yield an improved result over the CB.

Mention ought to be made of the target polarization which is also important particularly at low energies. Incorporation of this effect might be a step towards improvement of the CBO results.

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Note Added in Proof

In course of a discussion at the Paris ICPEAC with one of us (NCS) Tully has said that his remark in J. Phys. B is not in order. In fact he has not exactly repeated the calculation of Sural and Sil in the sense that he has used not the 2^1S wave function of Morse *et al* but that modified by him so as to make it orthogonal to the ground state function. By repeating the calculation with the 2^1S state function of Morse *et al* in its original form Tully has obtained in the partial wave method now a threshold cross section which is close to the value given by Sural and Sil.